Supplementary Material

to

The aggregation behaviour of 2*H*-imidazole-2-thione derivatives in solution, the solid state and over polycrystalline gold surface

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STable 1

Vibration assignation in the IR spectra recorded in the solid phase

Vibrations	Compounds			Vibration mode	Ref.
	1	**2**	**3**		
3089	+	+	+	νCH (sp^2)	[1]
2931	+	+	+	νCH (sp^3)	[2]
1657	+	–	+	δN–C	[3,4]
1496	+	+	+	δN–H/νC=N	[5–7]
1347	+	+	+	νC–N	[8]
1244	+	+	+	δCH_2–S	[9]
797	+	+	+	δring(imidazole) vibration	[10]
687	–	+	–	δring vibration	[11]

STable 2

Vibration assignation in the IR spectra recorded in solution

Vibrations	Compounds			Vibration mode	Ref.
	1	**2**	**3**		
~3250	+	+	+	νCH (sp^2) + νCH (sp^3)	[1,2]
~1600	+	+	+	δN–C	[3,4]
1350	+	+	+	νC–N	[8]
1318	+	+	+	δCH_2–S	[9]

Table 3

Raman shift assignation in the Raman spectra recorded in the solid phase

Vibrations	Compounds			Vibration mode	Ref.
	1	**2**	**3**		
3046	+	+	+	νCH (sp^2)	[1]
2965	+	+	+	νCH (sp^3)	[2]
1650	+	+	+	νC=C + νC=N	[12–15]
1600	+	–	–	νC=C + δN–H	[12–15]
1400	+	–	–	νC–N	[16]
1270	+	+	+	νC=S	[17]

Table 4

Raman shift assignation in the Raman spectra recorded in solution

Vibrations	Compounds			Vibration mode	Ref.
	1	**2**	**3**		
3035	+	+	+	νCH (sp^2)	[1]
1660	+	+	+	νC=C + νC=N	[12–15]
1490	+	+	+	νC–N	[16]
1442	+	+	+	νC=S	[17]

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